Computational Cosmology at Argonne National Laboratory

HEP staff: Salman Habib*, Katrin Heitmann*, Steve Kuhlmann
ALCF staff: Tim Williams (Mira Early Science Project)

HEP post-docs: Suman Bhattacharya*, Rahul Biswas, Sanghamitra Deb*, Juliana Kwan*, Adrian Pope*, Amol Upadhye*,
ALCF post-docs: Joe Bernstein, Hal Finkel (ESP)*

ALCF Student: Brittney Bullis (ESP)*

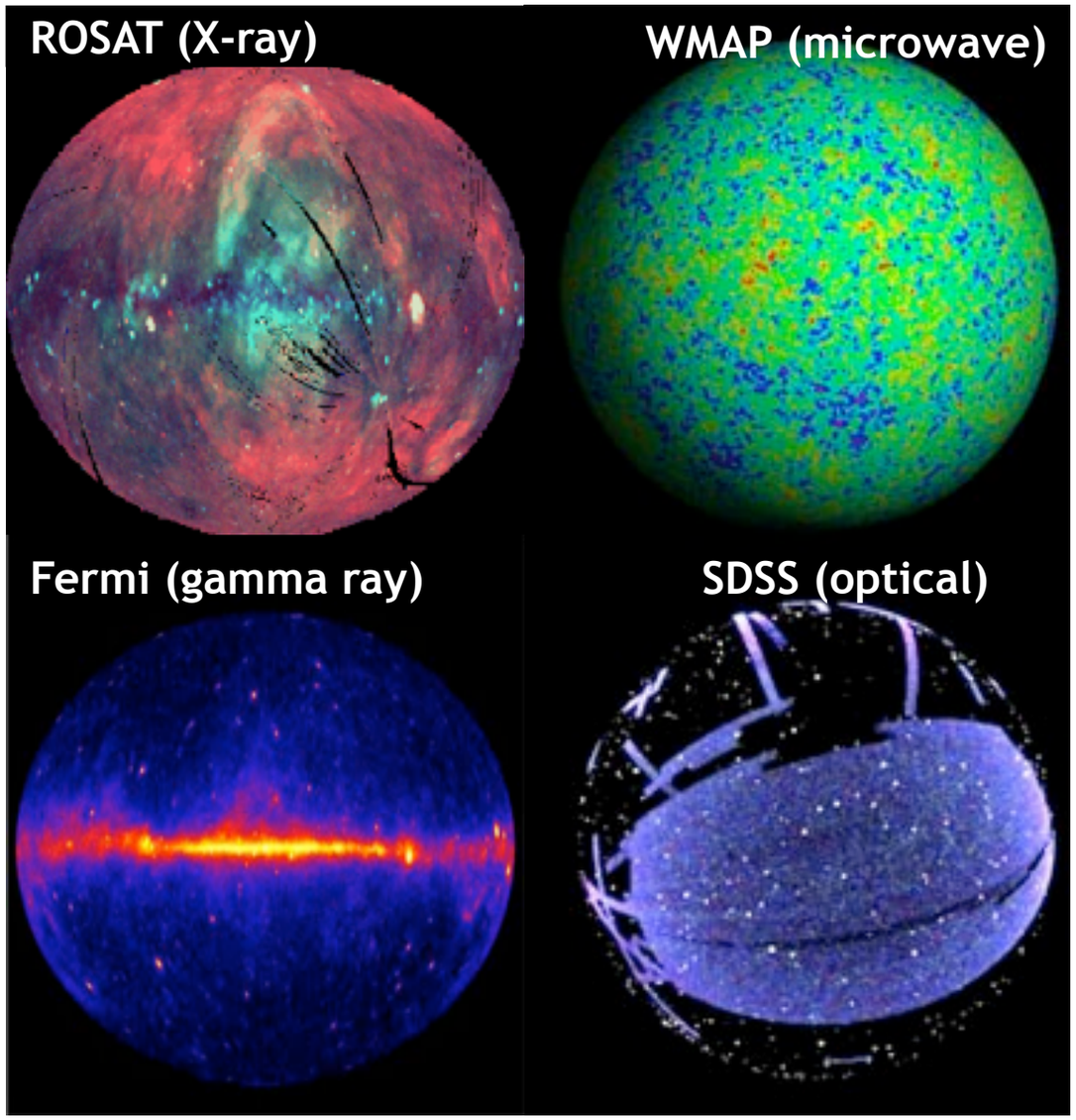
*recent/near-future arrivals

Collaborations and Projects

Kev Abazajian, Jim Ahrens, Ujjaini Alam, Debbie Bard, Sergei Bashinsky, Andrew Benson, Gary Bernstein, Joe Bernstein, Suman Bhattacharya, Derek Bingham, Rahul Biswas, Anna Cabre, Jordan Carlson, Joanne Cohn, Andrew Connolly, David Daniel, Nehal Desai, Scott Dodelson, Tim Eifler, Gus Evrard, Patricia Fasel, Hume Feldman, Wu Feng, Josh Frieman, Salman Habib, Katrin Heitmann, David Higdon, Tracy Holsclaw, Chung-Hsing Hsu, Bhuvnesh Jain, Steve Kahn, Lloyd Knox, Savvas Koushiappas, Juliana Kwan, Steve Kuhlmann, Earl Lawrence, Herbie Lee, Adam Lidz, Zarija Lukic, Chris Miller, Charles Nakhleh, Mike Norman, Alex Pang, Adrian Pope, Uliana Popov, Darren Reed, Paul Ricker, Robert Ryne, Bruno Sanso, Paul Sathre, Michael Schneider, Sergei Shandarin, Alex Szalay, Tony Tyson, Amol Upadhye, Licia Verde, Alexei Vikhlinin, Christian Wagner, Mike Warren, Martin White, Brian Williams, Jon Woodring, ---

Cosmological Probes of Physics Beyond the Standard Model

- **Dark Energy:** Properties of DE equation of state, modifications of GR, other models?
  Sky surveys, terrestrial experiments
- **Dark Matter:** Direct/Indirect searches, clustering properties, constraints on model parameters
  Sky surveys, targeted observations, terrestrial experiments
- **Inflation:** Probing primordial fluctuations, CMB polarization, non-Gaussianity
  Sky surveys
- **Neutrino Sector:** CMB, linear and nonlinear matter clustering
  Sky surveys, terrestrial experiments

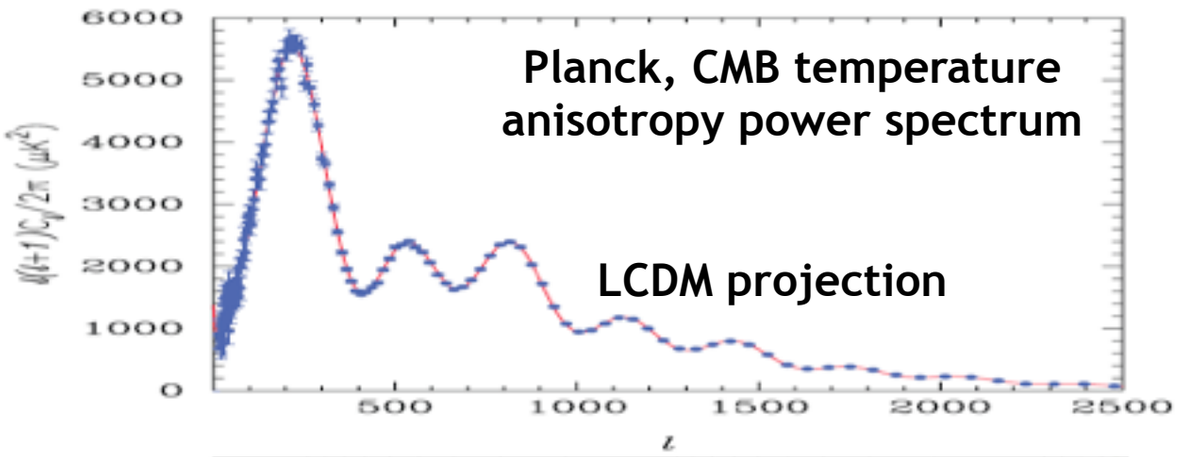


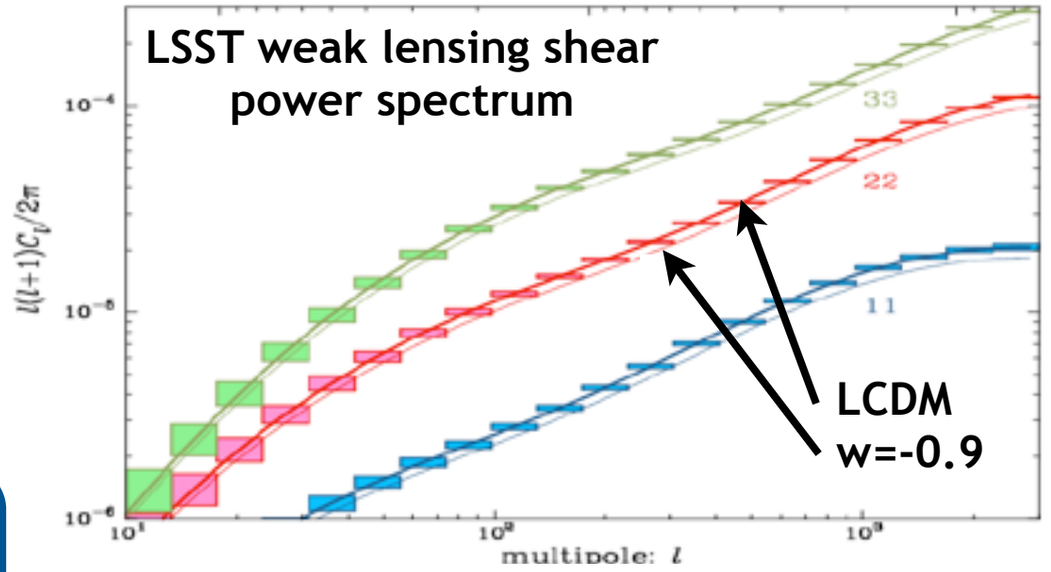
Explosion of information from sky maps: Precision Cosmology

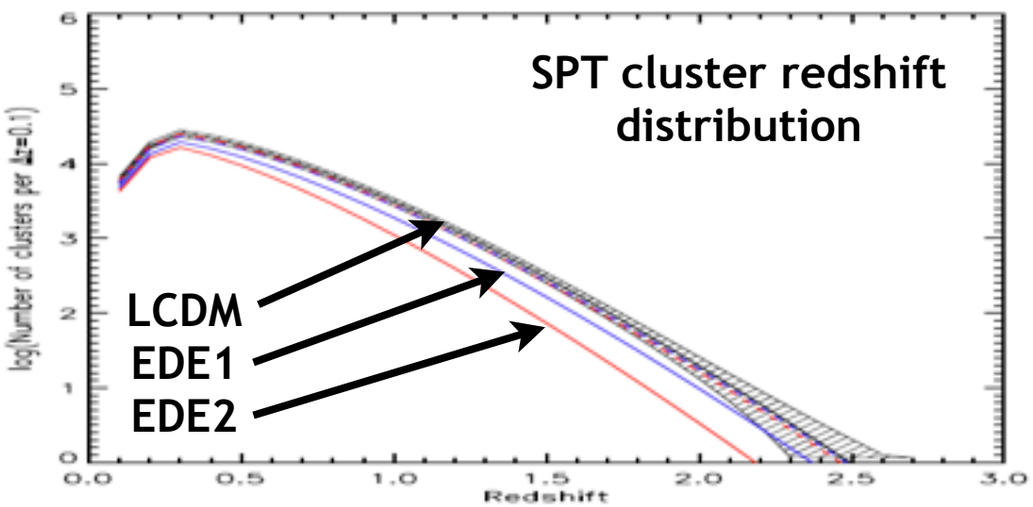
Precision Cosmology: "Inverting" the 3-D Sky

- **Cosmic Inverse Problem:** From sky maps to scientific inference
- **Cosmological Probes:** Measure geometry and presence/growth of structure (linear and nonlinear)
- **Examples:** Baryon acoustic oscillations (BAO), cluster counts, CMB, weak lensing, galaxy clustering, --
- **Standard Model:** Verified at the 5-10% level across multiple observations

- **Future Targets:** Aim to control survey measurements to the ~1% level
- **The Challenge:** Theory and simulation must satisfy stringent criteria for inverse problems and precision cosmology not to be theory-limited!

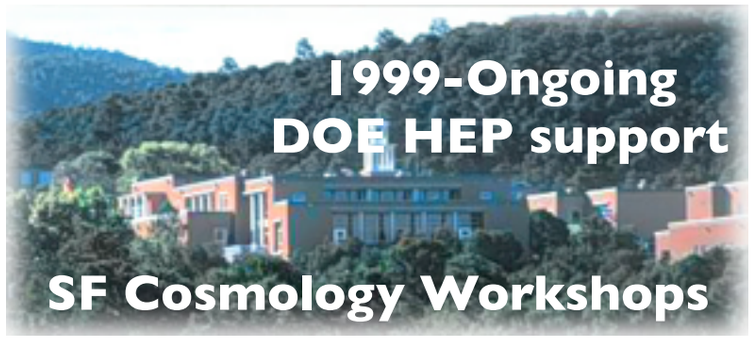


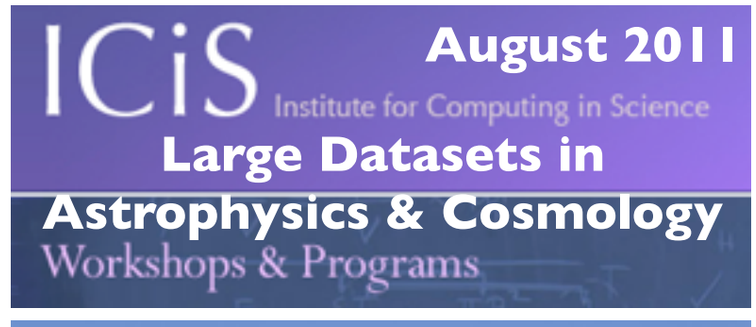




Getting Ready for the 'Great Surveys'

- **Community Effort Needed**
  - Lab-University teams/partnerships
  - Public release(s) of results and tools
- **New Generation of Simulations Necessary**
- **Active Interaction of Simulations with Data**
- **ANL Collaboration Examples:**
  - 'Chicagoland' Computational Cosmology Plan (ANL+U Chicago+Fermilab, report in June)
  - LSST/DES catalogs (Caltech, UC Berkeley/LBNL, SLAC/Stanford, Swinburne, U Washington, ---)
  - Weak Lensing (UC Berkeley/LBNL, U Chicago, Fermilab, Ohio State, U Penn, SLAC/Stanford, ---)
  - LSST 'end-to-end' modeling (UC Davis, LLNL, Purdue U, U Washington, ---)
  - DISC and large datasets (JHU, IPAC, NCSA, ---)



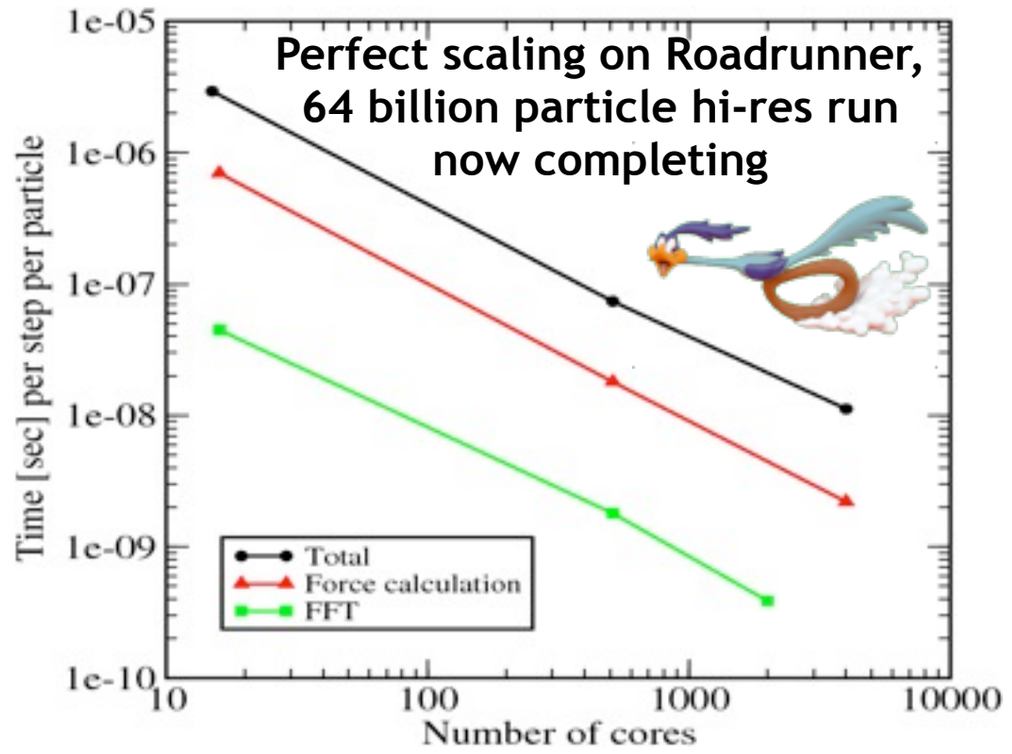


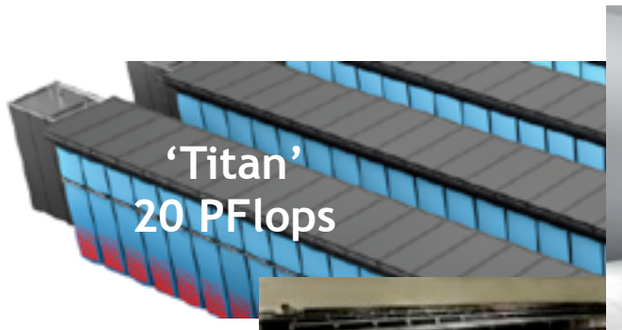
Computing the Universe: Simulating Surveys

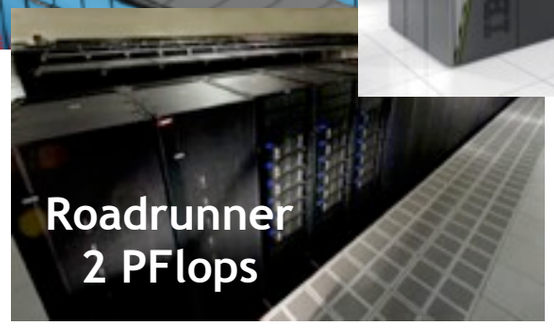
- **Simulation Volume:** Large survey sizes impose simulation volumes ~ (3 Gpc)^3, with memory requirements ~100 TB
- **Number of Particles:** Mass resolutions depend on ultimate object to be resolved, ~10^8 --10^{10} solar masses, N~10^{11}--10^{12}
- **Force Resolution:** ~kpc, yields a (global) spatial dynamic range of 10^6
- **Hydrodynamics/Sub-Grid Models:** Phenomenological treatment of gas physics and feedback greatly adds to computational cost
- **Throughput:** Large numbers of simulations required (100's --1000's), development of analysis suites, and emulators; peta-exascale computing exploits
- **Data-Intensive-SuperComputing:** End-to-End simulations and observations must be brought together in a DISC environment (theory-observation feedback)

Hardware-Accelerated Cosmology Code (HACC) Framework

- **Architecture Challenge:** HPC is rapidly evolving (clusters/BG/CPU+GPU/MIC --)
- **Code for the Future:** Melds optimized performance, low memory footprint, embedded analysis, and scalability
- **Implementation:** Long/short-range force matching with spectral force-shaping (long-range=PM, short-range=PP, tree)
- **Key Features:** Hybrid particle/grid design, particle overloading, spectral operators, mixed-precision, node-level 'plug-ins', ~50% of peak Flops
- **Cross-Platform:** Designed for all current and future supercomputing platforms
- **Embedded Analysis:** High performance with low I/O and storage requirement



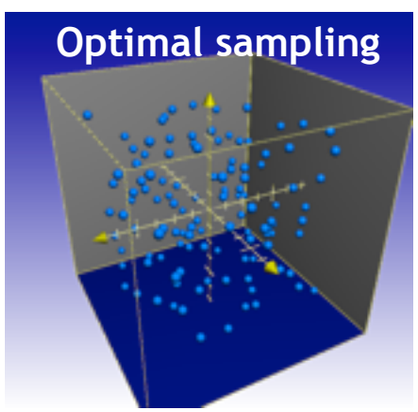


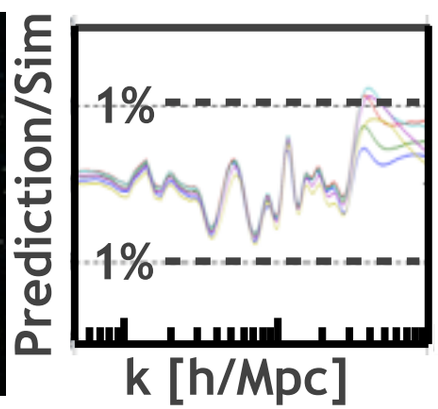


Habib et al. 2009, Pope et al. 2010

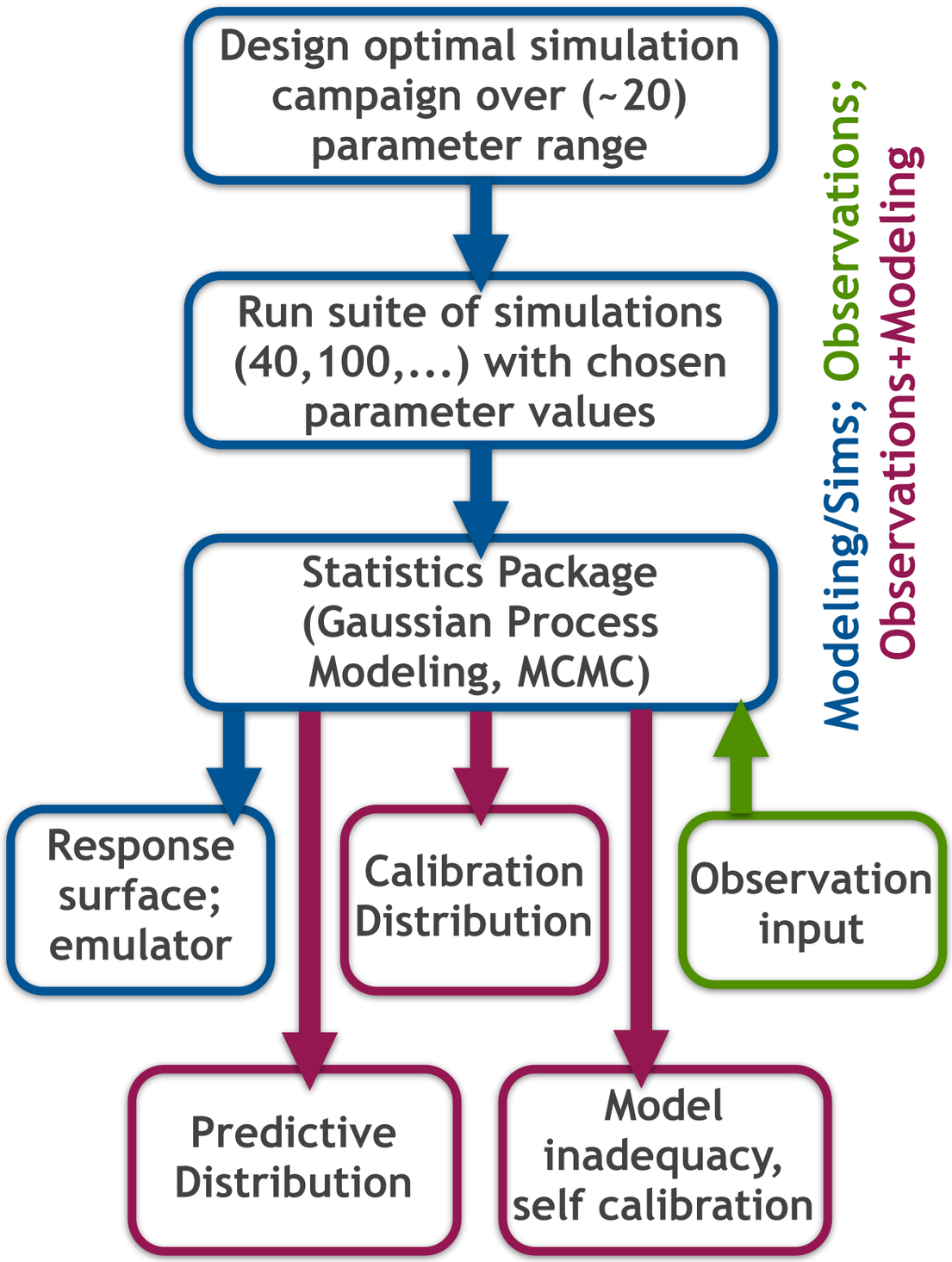
Cosmic Calibration: Solving the Inverse Problem

- **Challenge:** To extract cosmological constraints from observations in the nonlinear regime, need to run Markov Chain Monte Carlo; input: 10,000 - 100,000 different models
- **Brute Force:** Simulations, ~30 years on 2000 processor cluster ---
- **Current Strategy:** Fitting functions, e.g. for P(k), accurate at 10% level, not good enough!
- **Our Solution:** Precision emulators





Heitmann et al. 2006, Habib et al. 2007



Cosmic Emulator in Action

- Instantaneous ‘oracle’ for nonlinear power spectrum, easy to use, reduces run time from weeks to ‘zero’, 1% accurate to k~1/Mpc for wCDM cosmologies -- based on ~1000 simulation runs for 38 cosmologies
- For the first time enables direct MCMC with results from full simulations

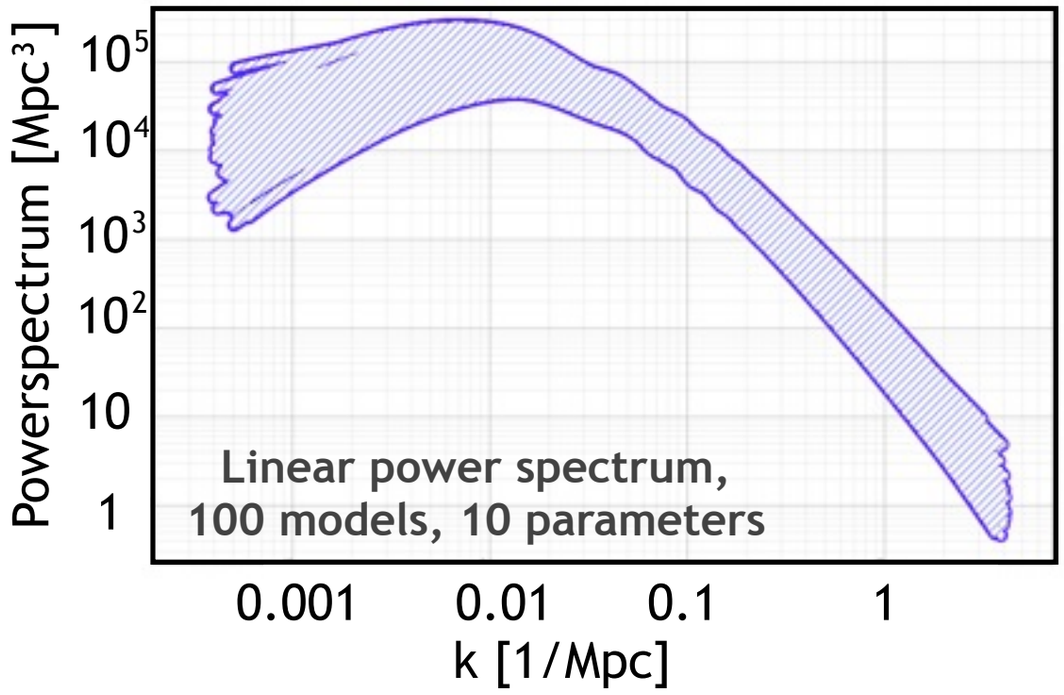
Cosmic Emulators for Future Surveys

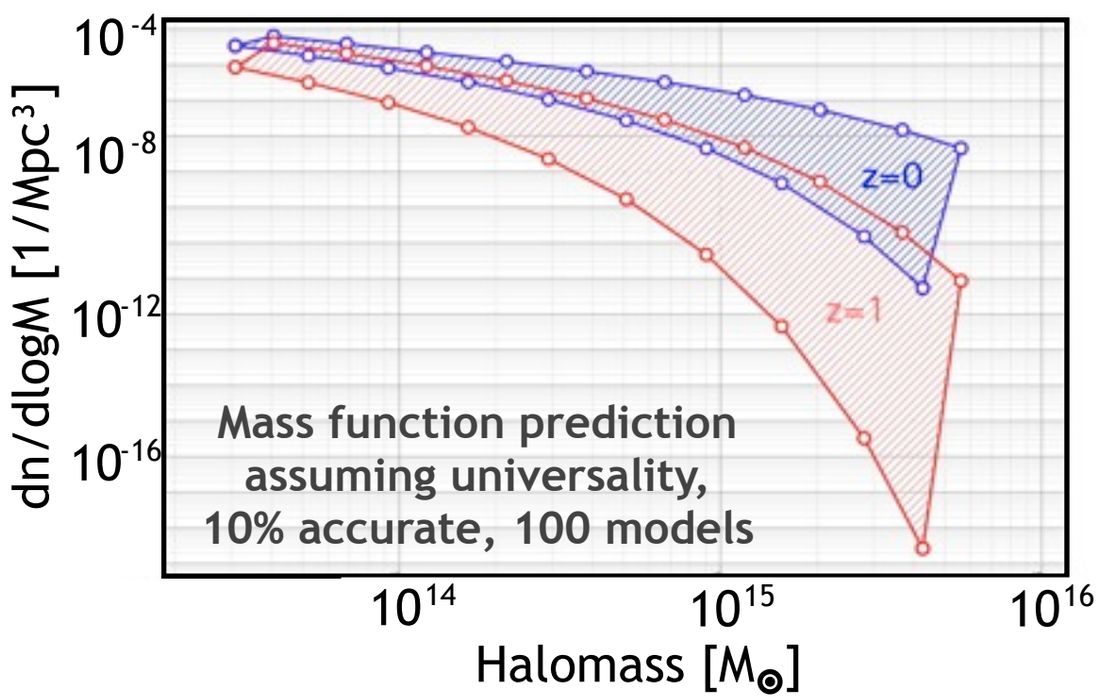
- **Extension Beyond wCDM:**

$$\theta = \{\omega_m, \omega_b, n_s, w_0, \sigma_8,$$
$$w_a, dn_s/d\log k, h, \Omega_k, f_\nu\}$$

Currently fine-tuning number of models and parameter ranges with surrogates, input from community

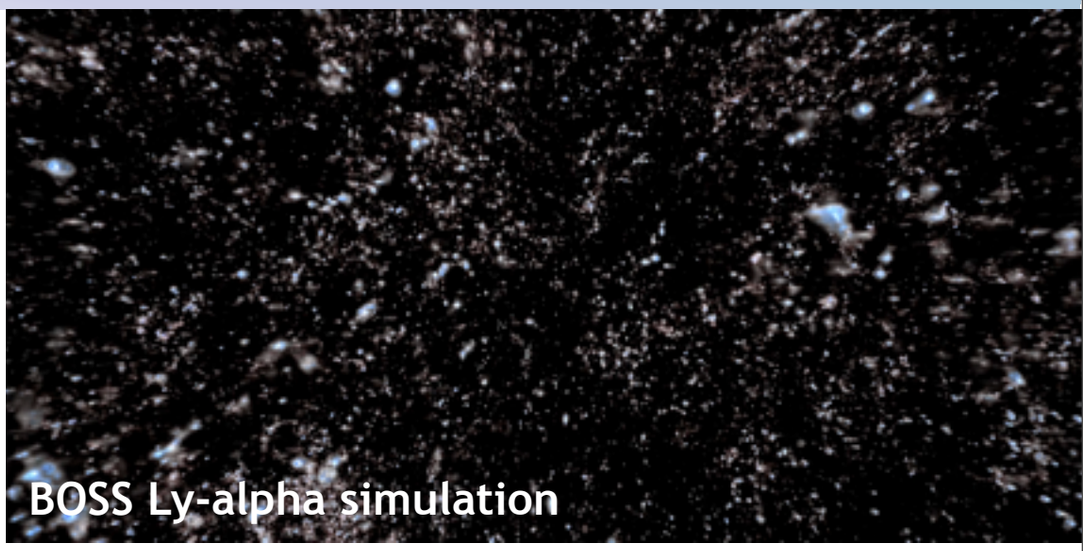
- **Emulators for a Variety of Observables:** power spectrum, mass function (different mass definitions), shear power spectrum, peak statistics, bias, ---
- **Extension of Range of Validity and 'Self-Calibration':** Higher resolution, baryonic physics, sub-grid models
- **Covariances**



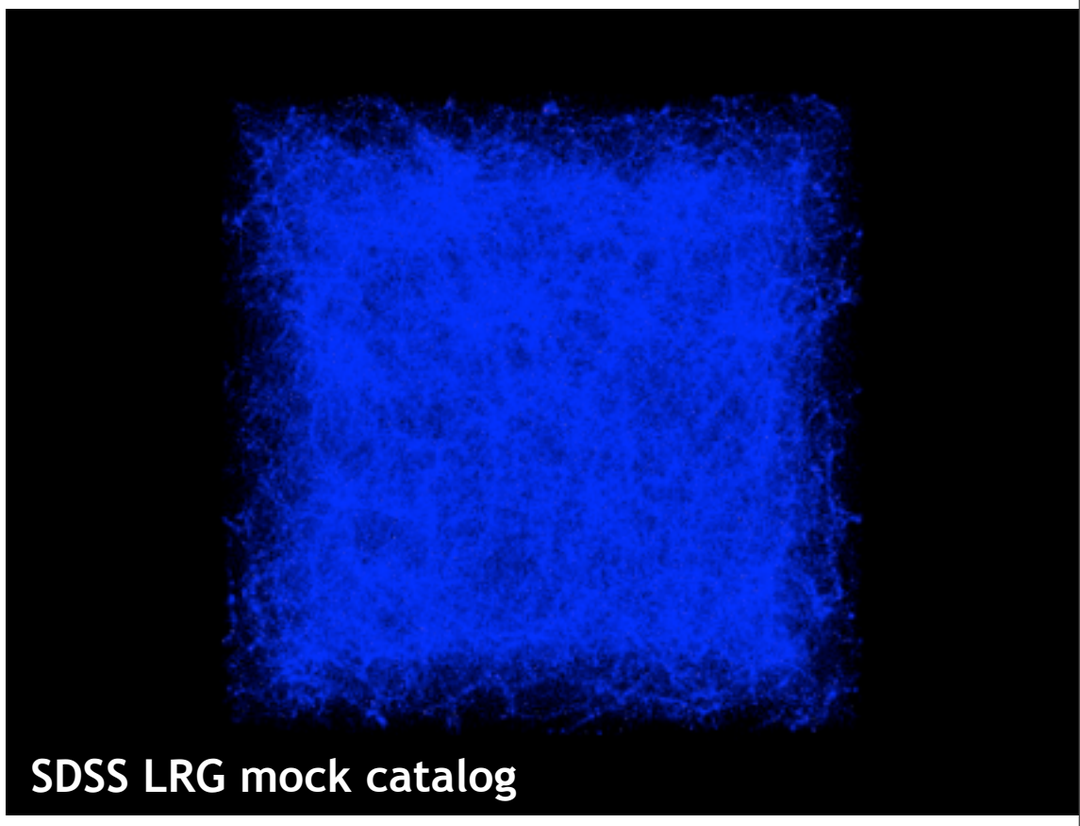


Summary and Outlook

- **HACC:** Up and running on GPU and Cell accelerated hardware
- **Cosmic Calibration:** Emulators enable solutions to inverse problems in the nonlinear regime
- **ESP on Mira:** 150M CPU hours, tree implementation almost completed, full-time post-doc and student
- **Hydrodynamics:** HACC optimal for particle-in-cell approach, algorithm development initiated, aim to complete by Mira arrival
- **HACC and Large Datasets:** Simulations and mocks need to be where the data is -- ANL provides state of the art resources via ALCF, Habib co-chair of now-forming Integrated System Simulation Working Group for LSST



Roadrunner view (halos) of the Universe at z=2 from a 64 billion particle run



Mock catalog for SDSS luminous red galaxies (orange) and satellite galaxies (green), in coll. with M. White